

1 **Quantifying the effects of gap on the molten pool and porosity formation in laser**
2 **butt welding**

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18
19 **Abstract**

20 To obtain a better joint quality in butt welding of aluminum, the gap filling process
21 and the quantification of the gap effects on the molten pool characteristic and the bubble
22 formation were realized by a three-dimensional thermal-mechanistic-fluid coupled
23 model, with the consideration of heat transfer, fluid flow, phase change and recoil
24 pressure. The model was validated by the synchrotron-radiation result. The competition
25 between the solidification and melting at the bottom of the molten pool was uncovered
26 to determine the gap filling process and the molten pool morphology. Gap increased the
27 heat loss, and the molten pool tip was elongated due to gap filling. Four phenomena
28 appeared in sequence in the initial stage of butt welding: I. Gap filling; II. Frozen; III.
29 Remelt; IV. Bubble formation. The result also demonstrated that the gap would disturb
30 the molten pool. In the initial stable growth stage of the molten pool, the larger the gap
31 width, the greater the molten pool depth. The sharp change of keyhole depth was due
32 to the necking formation, while the small fluctuation of keyhole depth with larger gap
33 values resulted from the perturbation by the gap. Bubble formation depends on the
34 degree of the fluid flow and the gap filling due to the unique fluid dropping down
35 phenomenon of butt welding with gap. A continuous melt pool cannot be formed when

36 the gap width beyond 20 μm , which is detrimental to the welding quality. These findings
37 are of great significance for guiding the optimization of butt-welding process, such as
38 reducing the roughness of the butt interface or increasing the clamping force to reduce
39 the butt gap.

40 *Keywords:* simulation; laser butt welding; gap filling; bubble

41 **1. Introduction**

42 Laser butt welding is increasingly adopted in the aerospace, automotive and
43 shipbuilding industries, which uses a moving laser beam as the heat source and joints
44 two parts by melting and solidification [1-3]. The interaction between laser and matter
45 accompanies by the rapid heating and cooling, involving many highly dynamic and
46 transient physical phenomena, such as melting, evaporation, molten metal flow,
47 solidification and non-equilibrium phase changes [4, 5], during which defects such as
48 pores and spattering may occur. To determine the optimal conditions and improve the
49 welding quality, the molten pool behavior in the welding process needs to be further
50 studied. With the development of science and technology, the in-situ observation
51 method based on X-ray imaging technology is an effective way to obtain the
52 information inside the molten pool [6-9]. A lot of work has been done to investigate the
53 dynamics of keyhole and molten pool, spatter and pore in the laser welding [10-15].
54 Matsunawa et al. [16] studied the keyhole and molten pool dynamics via the high-speed
55 in-situ X-ray imaging. Heider et al. [13] revealed that the bubble generated at the tip of
56 the capillary is one mechanism to cause welding defects, such as ejections and pores.
57 The increased pressure inside the keyhole promotes it to expand and thus forming
58 spatter. Similar mechanism was also uncovered by Miyagi [10]. Kawahito et al. [11]
59 performed the X-ray imaging of the keyhole and molten pool, and demonstrated that
60 the upward flow in the molten pool behind the keyhole leading to melt ejections.

61 Nevertheless, most of the in-situ monitoring experiments about the molten-pool
62 dynamic characteristic were conducted on the bead-on-plate welding situation, which
63 is different from the laser butt welding that possesses a gap at the interface. The existing
64 one about laser butt welding is conducted by Wang et al. [17] who observed the melting
65 and filling process by X-ray phase contrast imaging. They revealed two unique features
66 of molten pool, which are different from those of the plate welding. The molten pool
67 and keyhole were initially observed in the position below the upper surface and then
68 expanded upwards and downwards due to gap filling effect. In contrast, the molten pool
69 in laser welding is formed in the upper surface and then grew upwards through heat

70 transfer. The other difference is that there are two boundaries in the laser butt gap
71 welding. However, due to highly transient laser-matter interaction and the limited time
72 resolution of the X-ray contrast method (~ 1 ms), the specific gap filling process remains
73 challenging to study. Hesse et al. [18] revealed that variation in gap distance during
74 welding would lead to process instability and stress concentrations, which could
75 adversely affect the service properties. It will be of great significance for improving the
76 welding quality to further explore the gap filling process and the effect of the gap on
77 the weld pool characteristics with higher precision.

78 Numerical simulation is an economical and effective method that has been widely
79 adopted in the research of molten-pool dynamic simulations in the presence of heat
80 transfer and fluid flow [9, 19-27]. Cho et al. [20] investigated the temperature
81 distribution characteristic of weld bead and molten flow by simplifying the multi-phase
82 problem into a single-phase problem using finite volume method (FVM). The fusion
83 zone shape predicted by the simulation result was in good agreement with the
84 experimental fusion zone profile. Ai et al. [23] studied the molten pool and keyhole
85 profile as well as the defect generation during the high-power laser welding by FVM.
86 They revealed that the main factor for spattering formation is the column and swelling
87 in the oscillation interface between melt pool and keyhole. Li et al. [22] carried out
88 research on the keyhole evolution and molten metal flow under different sub-
89 atmospheric pressures in the laser welding of aluminum based on the FVM. They
90 demonstrated that the larger keyhole opening and larger melt flow velocity under a
91 lower pressure is responsible for the reduction of porosity. Leung et al [9] also revealed
92 that the pore and keyhole formation mechanisms are driven by the mixing of high
93 temperatures and high metal vapor concentrations in the keyhole using a combination
94 of in situ X-ray imaging and high-fidelity multiphase simulation.

95 In this paper, a three-dimensional multi-physics model is established to explore the
96 gap filling mechanism in the laser butt welding of aluminum, with the consideration of
97 heat transfer, fluid flow, recoil pressure, Marangoni effect and solidification drag model.
98 The proposed model is validated against the high-speed synchronous radiation result.
99 We use such model quantified the temperature distribution, fluid flow, as well as the
100 effects of gap on the molten pool characteristic and bubble generation.

101 **2. Mathematical model and numerical simulation**

102 The plates used in the experiment have a high surface finish with surface roughness
103 between $3\ \mu\text{m}$ to $6\ \mu\text{m}$. Several simulations with different gap values ($0\ \mu\text{m}$, $8\ \mu\text{m}$,
104 $12\ \mu\text{m}$, $16\ \mu\text{m}$, $20\ \mu\text{m}$, $24\ \mu\text{m}$) were carried out while considering the slight warping

105 phenomenon during the clamping process, where the modelling results with a gap value
 106 of 12 μm matched well with that of the experimental tests. Based on these simulations,
 107 the effect of different gap values on the joint quality were further explored.

108 The interaction between high-power laser and material involves many physical
 109 phenomena, such as heat transfer, phase change, gas and fluid flow, plume generation,
 110 etc. The following assumptions are made to simplify the calculation. (1) Only consider
 111 the heat transfer between the material and surrounding environment, while the shielding
 112 gas is neglected; (2) The plume and vapor dynamics due to evaporation is ignored, but
 113 the recoil pressure is included; (3) The fluid is regarded as incompressible Newtonian
 114 fluid with laminar flow. Volume of fluid (VOF) method is adopted to trace the evolution
 115 of free surface, in which scalar value F is used to represent the volume fraction of the
 116 fluid in a mesh. $0 < F < 1$ denotes the gas-fluid interface.

117 2.1 Recoil pressure

118 Evaporation occurs in the area with temperature above boiling point under laser
 119 irradiation, accompanied by the recoil pressure exerted in the opposite direction of
 120 vapor ejection. It is proportional to the saturation pressure and increases exponentially
 121 with the temperature rising. The widely accepted recoil pressure expression is
 122 Clausius–Clapeyron equation [28], which is suitable for the situation that ambient
 123 pressure has no influence in the evaporation process. In this work, the modified recoil
 124 pressure P_r is adopted based on ref. [29] which takes the ambient pressure into
 125 consideration, expressed as:

$$P_r = P_s - P_{atm} \quad (1)$$

$$P_s = \begin{cases} P_{atm} & 0 \leq T < T_{b1} \\ 0.002726506 * (T - 2606)^2 + 101300 & T_{b1} \leq T < T_{b2} \\ \frac{1 + \beta_R}{2} P_{atm} \exp\left[\frac{L_v(T - T_b)}{TRT_b}\right] & T_{b2} \leq T < \infty \end{cases} \quad (2)$$

126 here P_s is the surface pressure and P_{atm} is the ambient pressure. β_R is the
 127 recondensation coefficient and L_v denotes the latent heat of evaporation. T and T_b
 128 represent the liquid temperature and boiling point, respectively. R is the universal gas
 129 constant. T_{b1} and T_{b2} are defined as $0.95T_b$ and $1.05T_b$, respectively.

130 2.2 Heat source and boundary conditions

131 To be consistent with the experimental conditions, the laser beam is operating

132 continuous wave with a wavelength of 1060 nm. It is regarded as Gaussian distribution
 133 and a part of the surface heat flux boundary condition [30], described as

$$q = \frac{3PA}{\pi r^2} e^{\left[\frac{-3(x^2+y^2)}{r^2} \right]} \quad (3)$$

134 where q is the laser heat source, P is the laser power, A is the laser absorptivity
 135 value and r is the radius of the laser beam spot. (x, y) is the coordinate of the mesh
 136 within the laser irradiation. The algorithm for free-surface tracing is to find the mesh in
 137 the free surface under laser irradiation and heat it. After the time step, Δt , it repeats the
 138 above step until the calculation is ended. The energy transfer in the upper surface
 139 includes evaporation, radiation and convection. It can be expressed as

$$K \frac{\partial T}{\partial \vec{n}} = q - h_c(T - T_a) - \sigma \varepsilon (T^4 - T_a^4) - q_{evap} \quad (4)$$

$$q_{evap} = \varphi L_v P_{atm} \sqrt{\frac{1}{2\pi RT}} \exp \left[\frac{L_v(T - T_b)}{TRT_b} \right] \quad (5)$$

140 For other surfaces, only radiation and convection are considered. The balanced
 141 equation is

$$K \frac{\partial T}{\partial \vec{n}} = -h_c(T - T_a) - \sigma \varepsilon (T^4 - T_a^4) \quad (6)$$

142 Here K is the thermal conductivity and \vec{n} is the normal vector. h_c is the
 143 convective coefficient. T_a is the reference temperature and q_{evap} is the heat loss due
 144 to evaporation. φ is the accommodation coefficient. ε and σ represent the radiation
 145 emissivity and Stefan-Boltzmann constant, respectively. The balanced pressure
 146 boundary condition in the upper surface can be expressed by

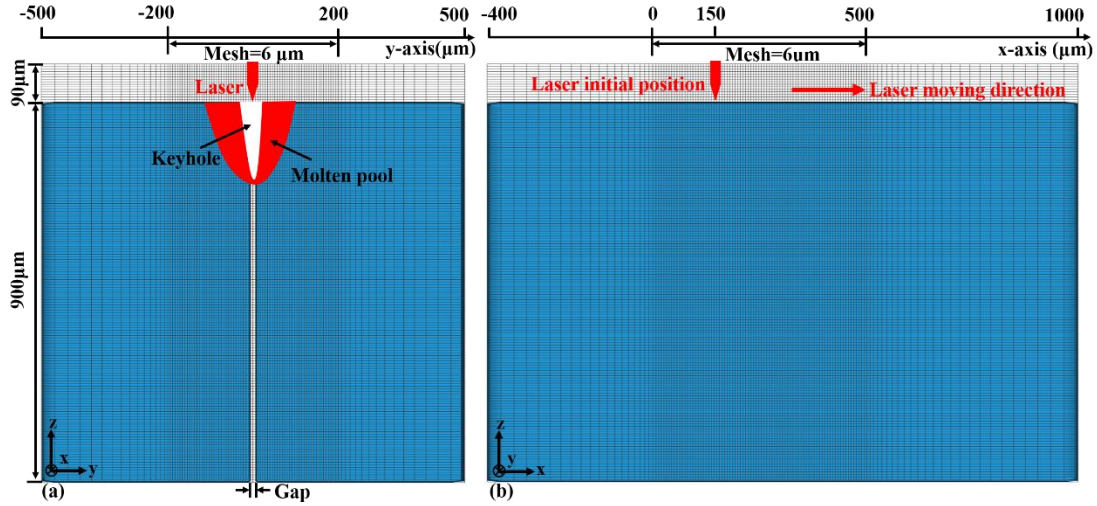
$$-P + 2\mu \frac{\partial \vec{v}_n}{\partial \vec{n}} = -P_r + \frac{\gamma}{R_k} \quad (7)$$

147 in which P is the pressure. μ and \vec{v}_n denote the viscosity and the normal velocity
 148 vector, respectively. γ is the surface tension and R_k is the radius of surface curvature.

149 2.3 Computational domain and simulation

150 The computational domain is shown in **Fig. 1**. In order to improve the
 151 computational efficiency without losing the accuracy, the mesh is divided in a non-
 152 uniform manner. It is set to be 6 μm along z-axis. The laser beam is located at $x=150$
 153 μm initially, moving along the positive direction of x-axis. The calculation time is set

154 to be 12 ms. In the region where a keyhole will form, the mesh is finely divided into 6
 155 μm . While out of this range, auto-mesh is applied by setting the mesh counts in a coarse
 156 manner to avoid the sharp change of mesh size. The total mesh count is > 2.1 million.



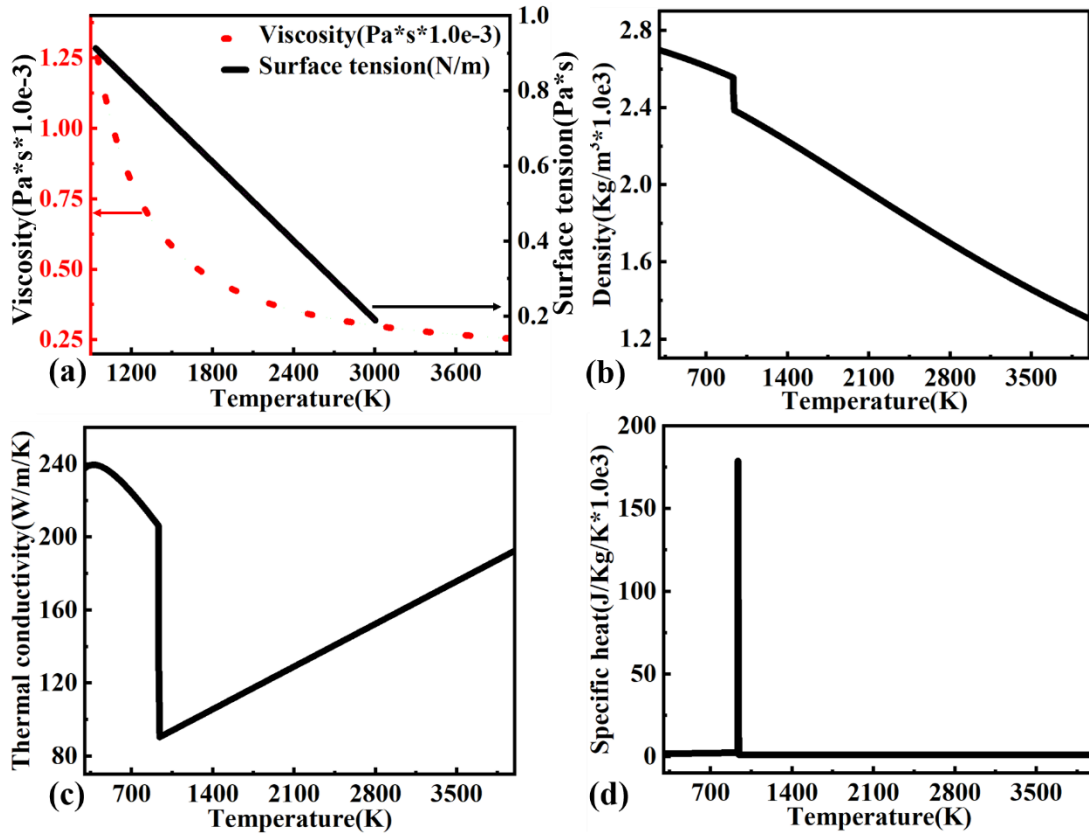
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158 **Fig. 1** Computational domain and mesh, (a) the left view, (b) the main view.

159 The simulation parameters can be found in **Table 1**. Laser power is 500 W and
 160 scanning speed is $16.7 \text{ mm} \cdot \text{s}^{-1}$. The laser spot diameter is $140 \mu\text{m}$. The thermophysical
 161 properties for aluminum are shown in **Fig. 2**. The temperature distribution, pressure and
 162 velocity in the molten pool can be obtained by solving the momentum conservation,
 163 energy conservation and mass conservation equations.

164 **Table 1** Parameters used in this simulation

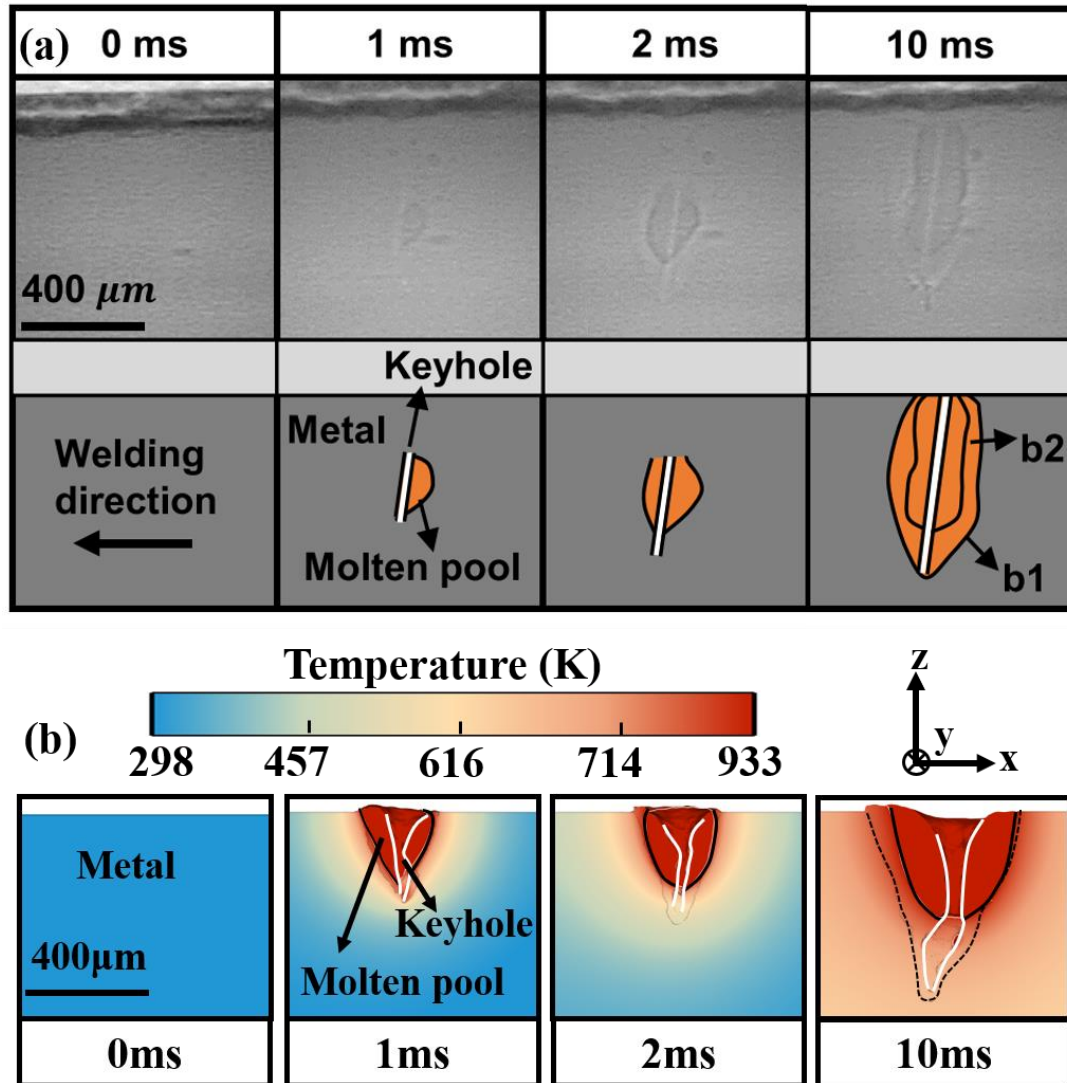
Properties	Value
Latent heat of evaporation L_v ($\text{J} \cdot \text{Kg}^{-1}$)	1.077E+07
Gas constant R ($\text{J} \cdot \text{Kg}^{-1} \cdot \text{K}^{-1}$)	308
Saturation pressure P_{atm} (Pa)	101300
Recondensation coefficient β_R	0.5795 [31]
Convective heat transfer h_c ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$)	80
Reference temperature T_a (K)	298
Stefan-Boltzman constant σ ($\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$)	5.67E-08
Radiation emissivity ε	0.36
Boiling temperature T_b (K)	2750
Melting temperature (K)	933
Absorptivity value A	0.65



165

166 **Fig. 2** Thermophysical properties for aluminum used in the simulation [32], (a)
 167 viscosity and surface tension, (b) density, (c) thermal conductivity, (d) specific heat.

168 The model is validated by comparing with the high-speed X-ray imaging results by
 169 Wang et al. [17], shown in **Fig. 3**. The simulated molten pool and keyhole morphology
 170 (500 W and $16.7 \text{ mm}\cdot\text{s}^{-1}$) are similar to those revealed by synchrotron radiations (500
 171 W and $16.7 \text{ mm}\cdot\text{s}^{-1}$), which validates the model.



172

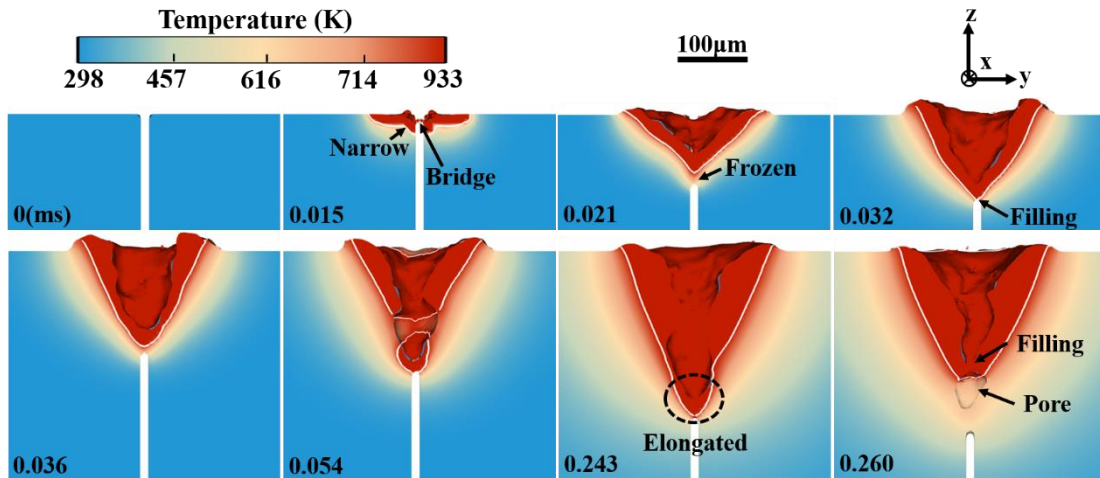
173 **Fig. 3** Simulation model validation, (a) X-ray imaging result (Reprinted from Ref. [17]
 174 with permission from Elsevier) and (b) simulation result. The solid white line shows
 175 the keyhole outline. The black solid and dotted lines in (b) represent the molten pool
 176 boundary and frozen line, respectively.

177 3. Results and discussion

178 3.1 Gap filling mechanism

179 The gap filling process and molten pool evolution are displayed in **Fig. 4**. At the
 180 initial stage (0.015 ms), a bridge is generated between two plates. The molten pool
 181 morphology initially presents two different ellipses, and the molten depth increases
 182 when approaching the gap. We hypothesize that those dynamics are induced by the
 183 downward fluid flows, driven by the gravity and recoil pressure, filling the gap. With
 184 the heat accumulation, the region adjacent to the gap absorbs much more energy,

185 leading to a triangular pyramid shape of the molten pool (0.021 ms). Under the effect
 186 of gap filling, the tip of molten pool is elongated and the corresponding depth rapidly
 187 increases. As the gap increases radiation, the fast downward flow reaches a deeper
 188 region and leads to a higher heat dissipation, causing fast solidification at the molten
 189 pool bottom. The frozen region (0.021 ms) prevents the downward filling, which is
 190 controlled by the competition between solidification, melting as well as the filling
 191 velocity. When the heat accumulates to a certain extent under the continuous laser
 192 irradiation, the frozen part remelts and the fluid continuously flows downward to fill
 193 the gap with an elongated tip (0.032 ms). Filling-solidification process repeats several
 194 times at the bottom of the molten pool, leading to necking formation in the upper part
 195 of the keyhole, blocking part of the laser energy. In the dual role of tip elongated and
 196 the necking, the lower part of the molten pool solidifies quickly while the keyhole
 197 sidewall is gradually captured by the solidification interface, resulting in a cut-off
 198 (0.054 ms). But the bottom can still be irradiated, and the keyhole depth still increases.
 199 After that a bridge forms between the rear and front keyhole wall, and a pore is
 200 generated at the bottom of laser-matter interaction zone (0.260 ms).

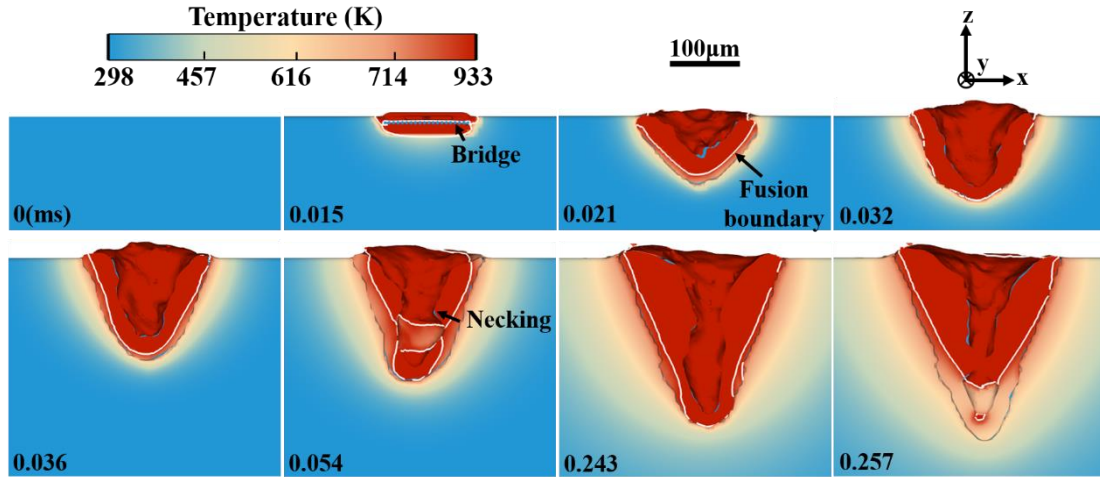


201

202 **Fig. 4** Evolution of molten pool and the gap filling process in the cross-section ($x=150$
 203 μm) perpendicular to the laser moving direction. The white lines denote the fusion
 204 boundary. The gap distance is $12 \mu\text{m}$.

205 **Fig. 5** shows the molten pool evolution and gap filling process in the cross-section
 206 view ($y=0 \mu\text{m}$) parallel to the laser moving direction. A bridge occurs between two
 207 plates at 0.015 ms, in which the length of the molten pool is smaller due to the gap
 208 filling effect. As the downward flow penetrates to a deeper region in the gap, the rapid
 209 radiation and heat conduction promote the fluid solidification and forming a frozen area
 210 (0.021 ms). The frozen part stops the fluid from filling the gap and decreases the heat

211 dissipation. The heat accumulated to some specific levels, the solidified region is
 212 remelted and the fluid flow downwards to fill the gap (0.032 ms). The filling-
 213 solidification process repeats continuously as the fluid flows downward to fill the gap
 214 during the expansion of the molten pool. As the keyhole depth grows further, necking
 215 is formed at the upper part of the keyhole, increasing the disturbance to the melt pool
 216 and keyhole (0.054 ms). At this stage, the keyhole is much more unstable, easily to form
 217 a bubble at the bottom (0.257 ms).



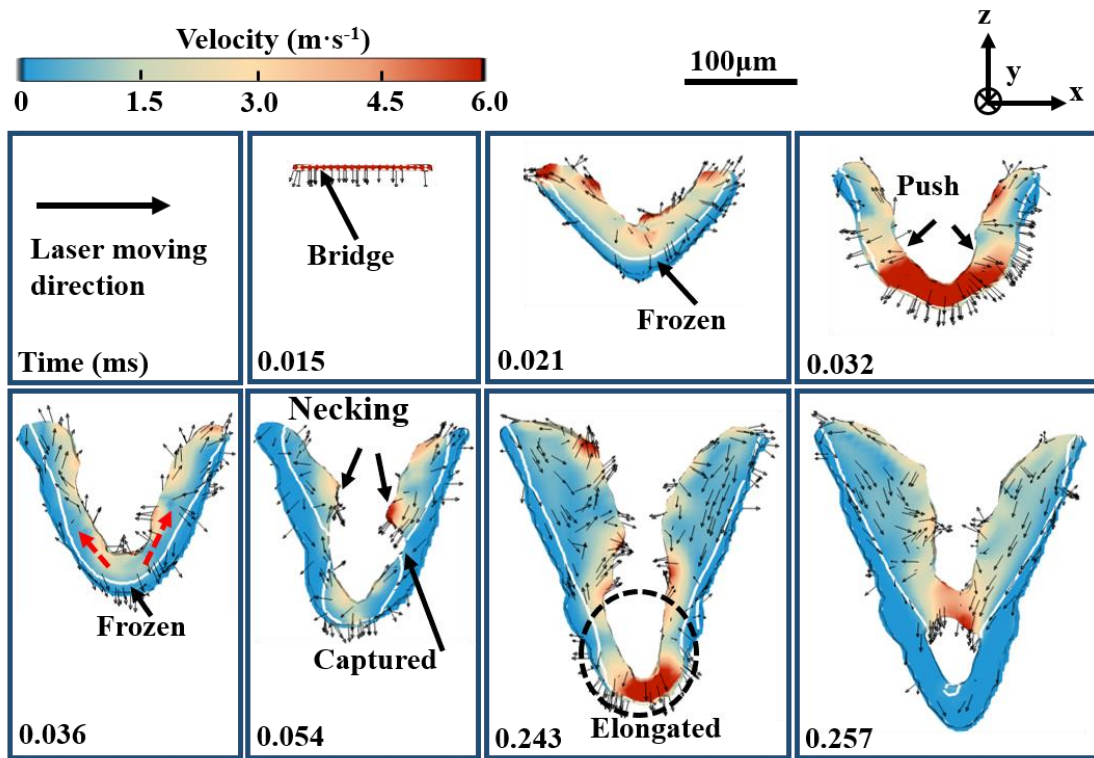
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219 **Fig. 5** Evolution of molten pool and the gap filling process in the cross-section parallel
 220 to the laser moving direction. These 3D temperature clips are located at $y=0 \mu\text{m}$ (the
 221 middle of the gap). The white lines denote the fusion boundary. The gap distance is $12 \mu\text{m}$.
 222

223 The fluid dynamics in the gap are presented in **Fig. 6**. The metal melts under the
 224 irradiation of laser, then flows downwards due to the gravity and recoil pressure. The
 225 fast heat dissipation at the molten pool bottom causes freezing. Then the fluid flows
 226 upward along the rear and front keyhole wall other than downward (0.021 ms). Under
 227 the continuous laser irradiation, the frozen part remelts and the molten pool depth
 228 increases. The fluid flows radially outward due to the recoil pressure and fills the gap
 229 (0.032ms), leading to the elongation of the melt pool tip. By repeating the gap filling-
 230 solidification process, the molten region gradually expands. When the keyhole drills
 231 down to an unstable state, necking occurs on the keyhole wall, causing fluctuation. The
 232 combination of tip elongated effect and necking results in the keyhole sidewall to be
 233 captured by the liquid-solid interface while the bottom can still get irradiation and melt
 234 (0.054 ms). Then a bridge forms between the rear and front keyhole wall and generates
 235 a bubble.

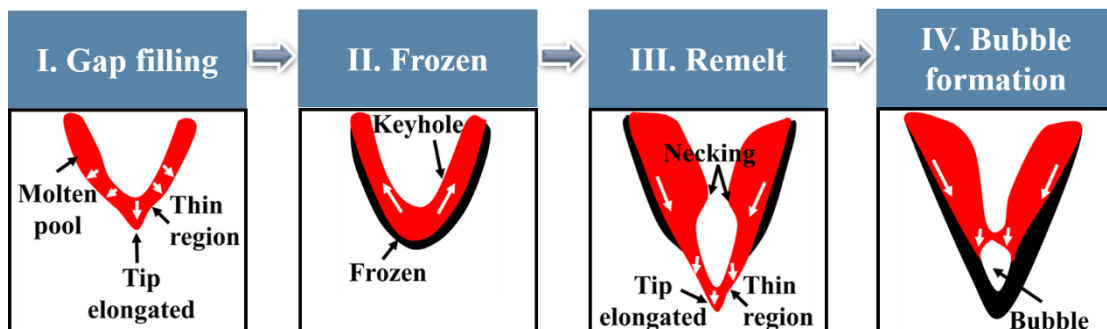
236 From the above discussion, there are four phenomena appearing in sequence in the

237 initial stage of welding, shown in Fig. 7. I. Gap filling: Molten metal forms and the
 238 melting velocity exceeds the solidification velocity, the fluid flows downward to fill the
 239 gap. II. Frozen: As the fluid flows reaching a certain depth where the heat dissipation
 240 is greater than the heat accumulation, namely, the solidification velocity is larger than
 241 both the melting and filling velocities, the molten pool bottom solidifies, preventing the
 242 downward flow and reducing the heat loss. III. Remelt: As the numerous heat
 243 accumulation, the melting process gradually dominates the solidification process, the
 244 fluid continuously flows downward and fill the gap. IV. Bubble formation: The filling-
 245 solidification process repeats. When the keyhole depth reaches an unstable state,
 246 necking occurs and promotes the keyhole fluctuation. Coupled with the tip elongated
 247 effect, the bubble is easily generated at the bottom of the keyhole.



248

249 **Fig. 6** Snapshots of the fluid flow in the gap. The white lines denote the fusion boundary
 250 and the gap width is 12µm.



251

252 **Fig. 7** Four key phenomena in the initial stage of welding. The white arrows denote the
253 fluid direction.

254 **3.2 Influence of gap on the filling process**

255 To explore the effect of gap on the joint quality, models with different gap values
256 are established, and the fluid flow, molten pool evolution and force distribution are
257 analyzed.

258 The evolution of molten pool and gap filling process are demonstrated in **Fig. 8**.
259 The laser beam moves along the positive direction of the x-axis. The top surface of the
260 material absorbs the laser energy and starts to melt when the temperature exceeds the
261 melting point. A bridge is formed between the two plates due to surface tension, which
262 is in the shape of an arch (0.015 ms). With large gap width, the gravity and recoil force
263 play a dominant role, and the fluid flows downward to fill the gap. The molten pool
264 depth close to the gap is large while that in the region far from the gap is small, and
265 there is a sharp change. The heat energy accumulates and conducts around, causing the
266 molten pool expanding. The surface tension decreases while the recoil force rises
267 exponentially with a higher temperature [33]. Under the effect of gap filling, the tip of
268 the molten pool is elongated, and the larger the gap, the longer it is stretched. Under the
269 same moment, the molten pool depth increases with a larger gap. At the time of 0.021 ms,
270 the bottom of the molten pool has solidified in the case with large gap width (12 μm
271 and 16 μm), preventing the gap filling. Under the condition with gap width being 8 μm ,
272 no solidification has occurred. This can be attributed to that the larger the gap, the more
273 heat loss by radiation; the deeper the molten pool, and the faster the heat conduction.
274 These combined effects cause the solidification speed to prevail and the freezing occurs.
275 It can be seen at the moment of 0.032 ms that the remelting for the case of 12 μm has
276 priority over the case with 16 μm . This is due to the larger heat dissipation requiring
277 more heat accumulation. While the molten pool depths for the models with gap width
278 0 and 8 μm gradually increase.

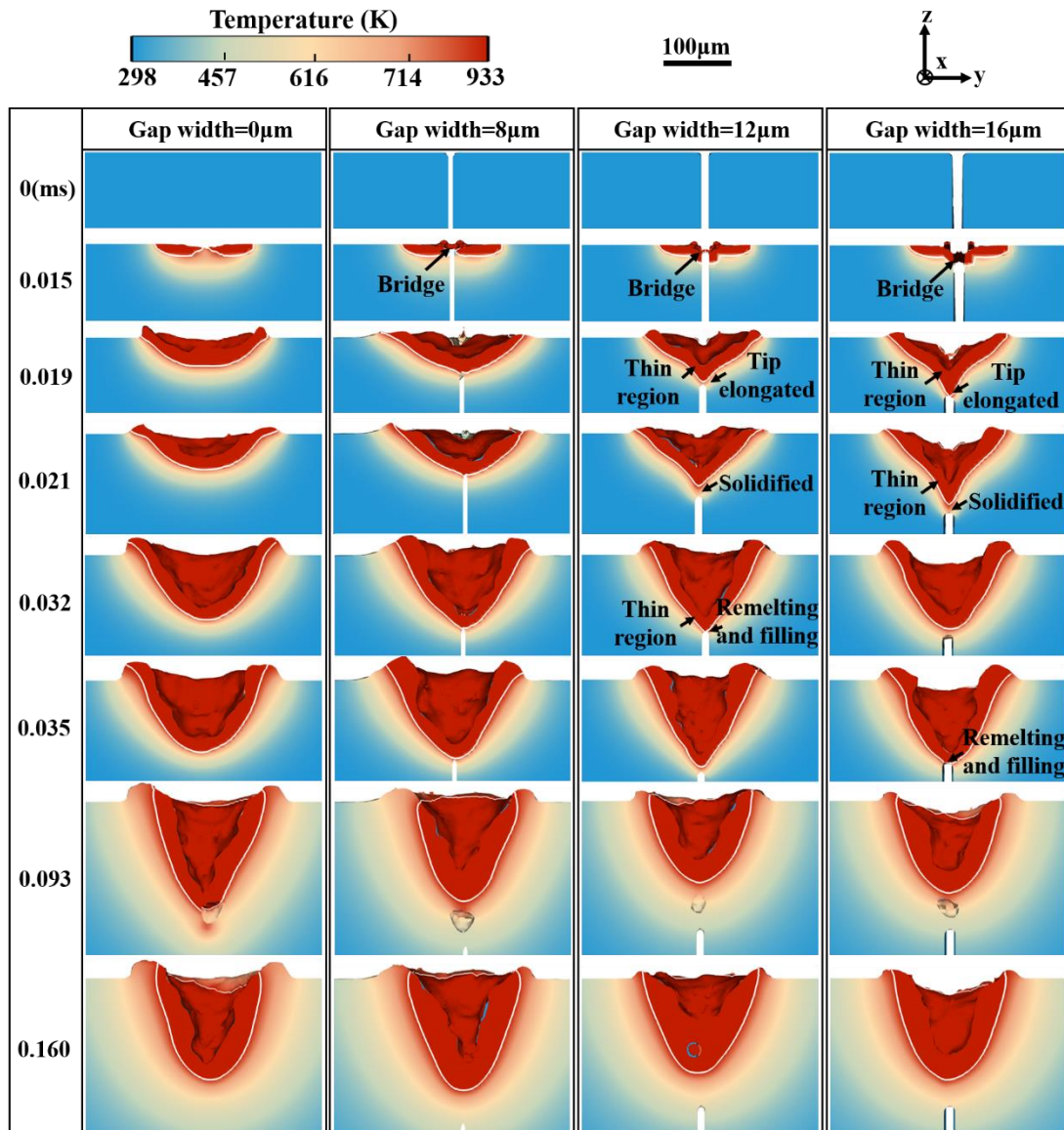
279 This filling-solidification process repeats and when the keyhole depth exceeds a
280 certain range, necking forms on the keyhole wall, causing fluctuation. Due to the effect
281 of gap filling, the tip of the molten pool is elongated, and the region between the keyhole
282 wall and the fusion boundary becomes thinner. Under the effects of the two, the tip of
283 the molten pool is more unstable and easily forms a bubble [7].

284 The velocity distribution of the fluid with different gap width is displayed in **Fig.**
285 **9**. As laser initially irradiates the material, the keyhole has not been formed and the fluid
286 velocity for the gap width 0 μm is near 0 $\text{m}\cdot\text{s}^{-1}$ (0.015 ms). The velocity increases with

287 the gap width rising, which can be attributed to more space for the fluid to flow. As the
288 time extends, keyhole gradually appears for the 0 μm case, around which the velocity
289 evenly distributes. While for the cases with a gap exists, the region closer to the gap
290 possess larger velocity due to the gap filling effect that melt drops down. At the moment
291 of 0.021 ms, the solidification dominates at the melt pool bottom for the 12 μm case.
292 Thus, the fluid cannot flow downward and the velocity decreases. For the case of 16
293 μm , despite the large heat dissipation, the filling effect still dominates the fluid flow
294 due to the large gap width. When it comes to the 0.032 ms, for the cases with small gap
295 values (0 μm and 8 μm), the low velocity leads to the melt pool expanding slowly. When
296 the gap width is 12 μm , the heat accumulation results in the melting and downward
297 filling prevailing. While for the case of 16 μm , the melt pool bottom just starts to
298 solidify, which is later than that of the 12 μm , and the velocity is close to 0 $\text{m}\cdot\text{s}^{-1}$. At the
299 moment of 0.093ms, the keyhole oscillation causes the bottom of the melt pool to
300 solidify and form pore, preventing the downward flow.

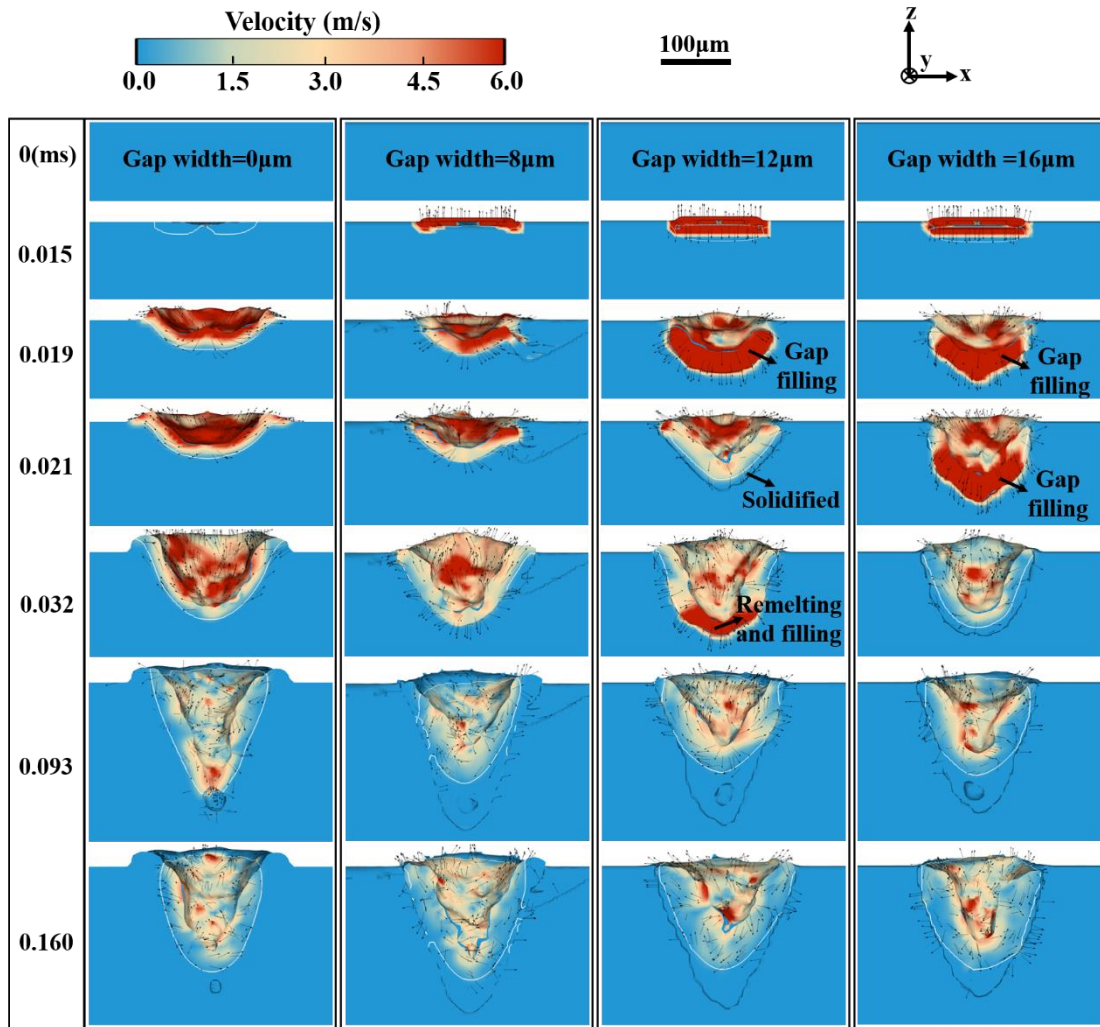
301 **Fig. 10** shows the snapshots of the molten pool morphologies with different gap
302 widths from the top view. In the presence of gap, a bridge occurs between two plates
303 due to the surface tension (0.015 ms). As the temperature increases, the recoil pressure
304 rises exponentially, radially outward. The larger the gap, the more the heat dissipation,
305 resulting in a smaller recoil pressure, which can be seen in **Fig. 11**. In the case of gap
306 width being 8 μm , spattering occurs due to the large recoil pressure (**Fig.11** (b)) at 0.019
307 ms. While for the models with larger gap width, the downward filling coupled with the
308 smaller recoil pressure, no obvious spatter happens. Under the effect gap filling, the
309 molten length is smaller than its width, while for the case with no gap, it is circular in
310 the top view. Actually, the gap filling process is somewhat similar to deep penetration
311 welding, not only the heat dissipation by radiation and conduction, but the direct energy
312 loss as the laser penetrates the plates [34].

313 In fact, we also explored larger gap width, shown in **Fig. 12**. However, the results
314 reveal that when the gap width exceeds 20 μm , the fluid will fall down during the gap
315 filling process. That is to say, a continuous melt pool will not be formed, which is not
316 conducive to the welding quality. These findings are of great significance for optimizing
317 the butt-welding process. Measures such as reducing the roughness of the butt interface
318 or increasing the clamping force can be adopted to reduce the butt gap and improve the
319 joint quality in the actual laser butt welding process.



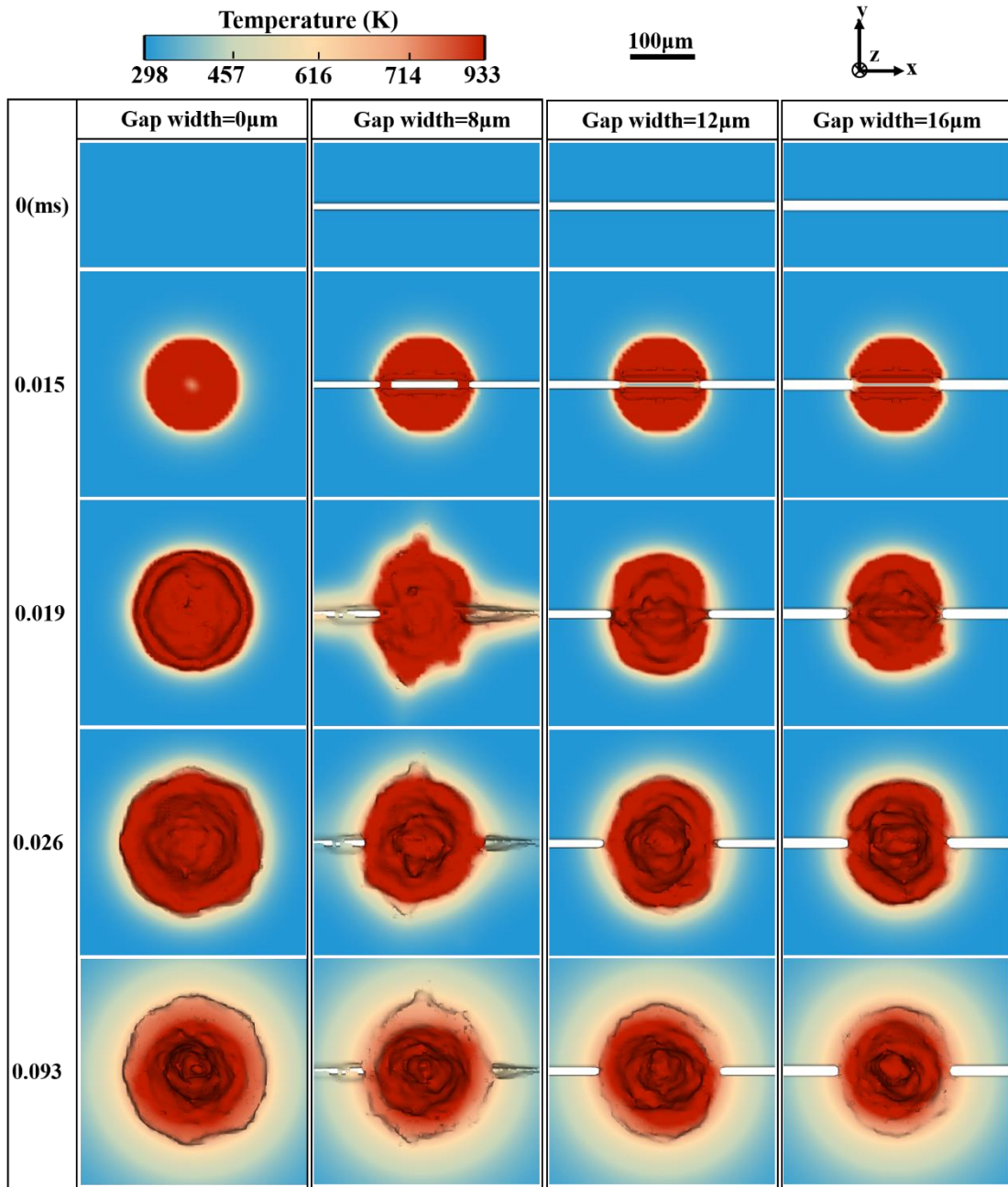
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321 **Fig. 8** Evolution of molten pool in the cross-section ($x=150 \mu\text{m}$) perpendicular to the
 322 laser moving direction with different gap values (0 -16 μm). The laser beam moves
 323 along the positive direction of x-axis. These 3D temperature clips are located at the
 324 middle of the gap.



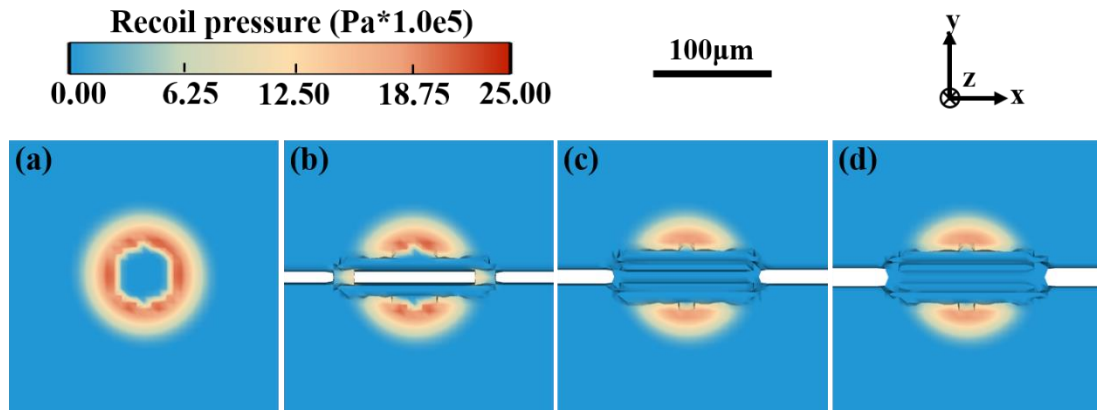
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326 **Fig. 9** Evolution of molten pool and the fluid flow in the cross-section ($x=150 \mu\text{m}$)
 327 parallel to the laser moving direction with different gap values (0 -16 μm). The laser
 328 beam moves from left to right. These 3D velocity clips are located at the middle of the
 329 gap.



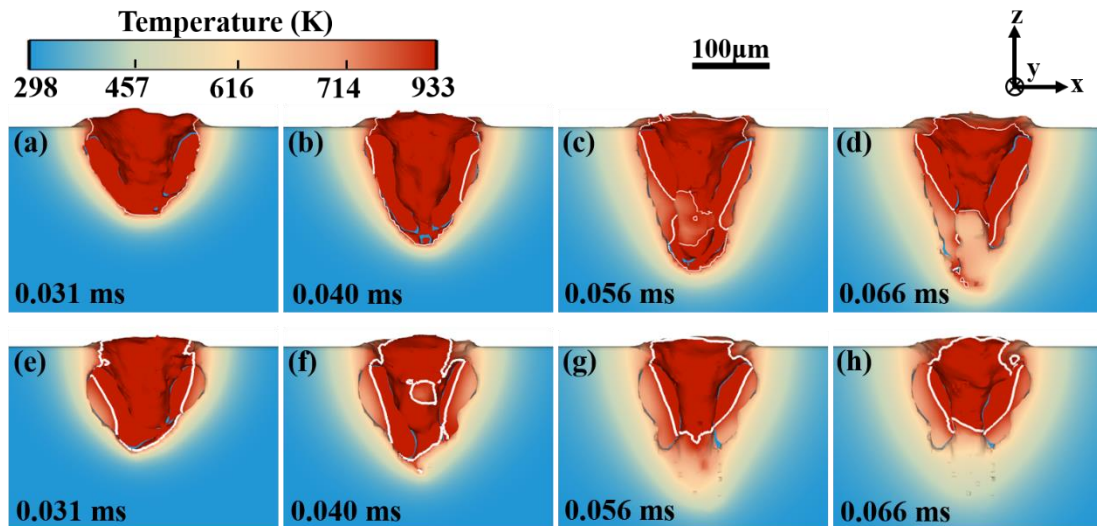
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331 **Fig. 10** Snapshots of molten pool morphology form the top view with different gap
 332 widths. The laser beam moves from left to right.



333

334 **Fig. 11** Distribution of recoil pressure with gap width being (a) 0 μm , (b) 8 μm , (c) 12
 335 μm and (d) 16 μm at 0.019 ms from the top view. The laser beam moves from left to
 336 right.



337

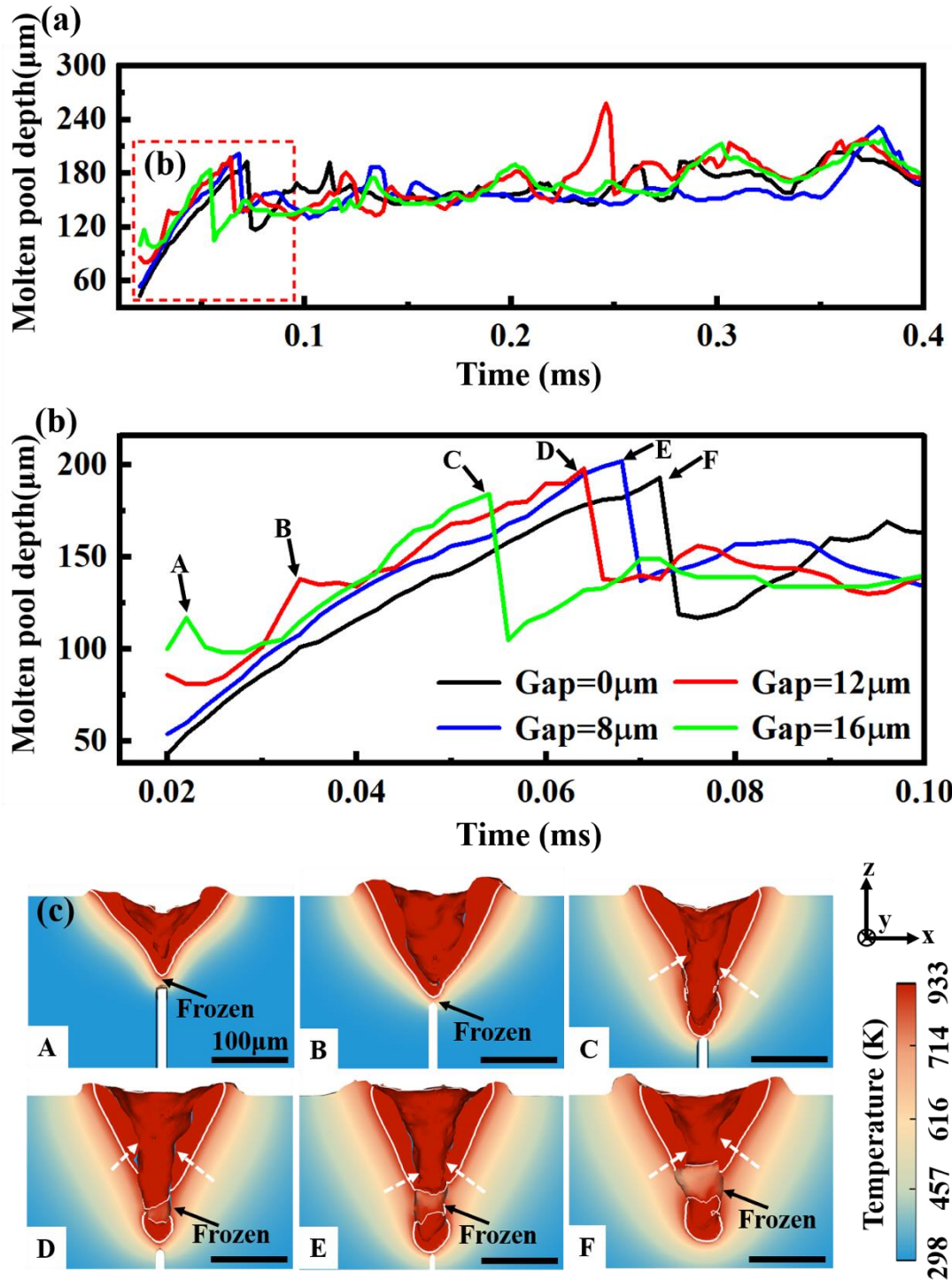
338 **Fig. 12** Evolution of molten pool in the cross-section parallel to the laser moving
 339 direction with gap width (a-d) 20 μm and (e-f) 24 μm . The laser beam moves from left
 340 to right. These 3D temperature clips are located at the middle of the gap.

341 3.3 Molten pool characteristic and pore generation

342 As the joint quality is affected by the stabilities of the molten pool and keyhole, in
 343 this part, the characteristic of the molten pool and bubble formation are studied. The
 344 depth of molten pool is plotted in **Fig. 13** and the profiles at specific points are also
 345 displayed.

346 In the initial stable growth stage of molten pool depth, the larger the gap width, the
 347 greater the depth under the same moment, which can be attributed to the gap filling

348 effect of melt dropping down. It can be seen from the enlarged picture in **Fig. 13** (b)
349 that in the first stage of the overall increase in the depth, there are some small fluctuation
350 points (A, B) in the case of 12 μm and 16 μm . This is because gap intensifies the heat
351 dissipation and solidification dominates, resulting in the depth decreasing. Due to the
352 heat accumulation, the frozen region remelts and the depth rises, indicating that the
353 existence of gap disturbs the molten pool. As the gap filling leads to the elongation of
354 molten pool tip, a thin region between keyhole wall and fusion line was induced (**Fig.**
355 **8**). Under the dual action of gap disturbance and keyhole fluctuation, the case with
356 largest gap width starts to solidify in the first place, decreasing the molten pool depth,
357 and the stable growth stage ends. The smaller the gap, the larger the depth achieved in
358 the first stage. This can be attributed to the low heat dissipation and large heat
359 accumulation. The depth for 0 μm is lower than that of 8 μm , because gap = 8 μm
360 possesses the advantages of small heat dissipation and gap filling effect, resulting in a
361 larger depth. A and B represent the fluctuation of melt pool depth caused by the large
362 gap. C-F indicate the perturbation to the melt pool due to the keyhole instability in all
363 cases, leading to a sharp change in the depth of molten pool. The larger the gap, the
364 earlier the perturbation occurs. Although the existence of gap also has an effect on the
365 depth, the change is smaller.



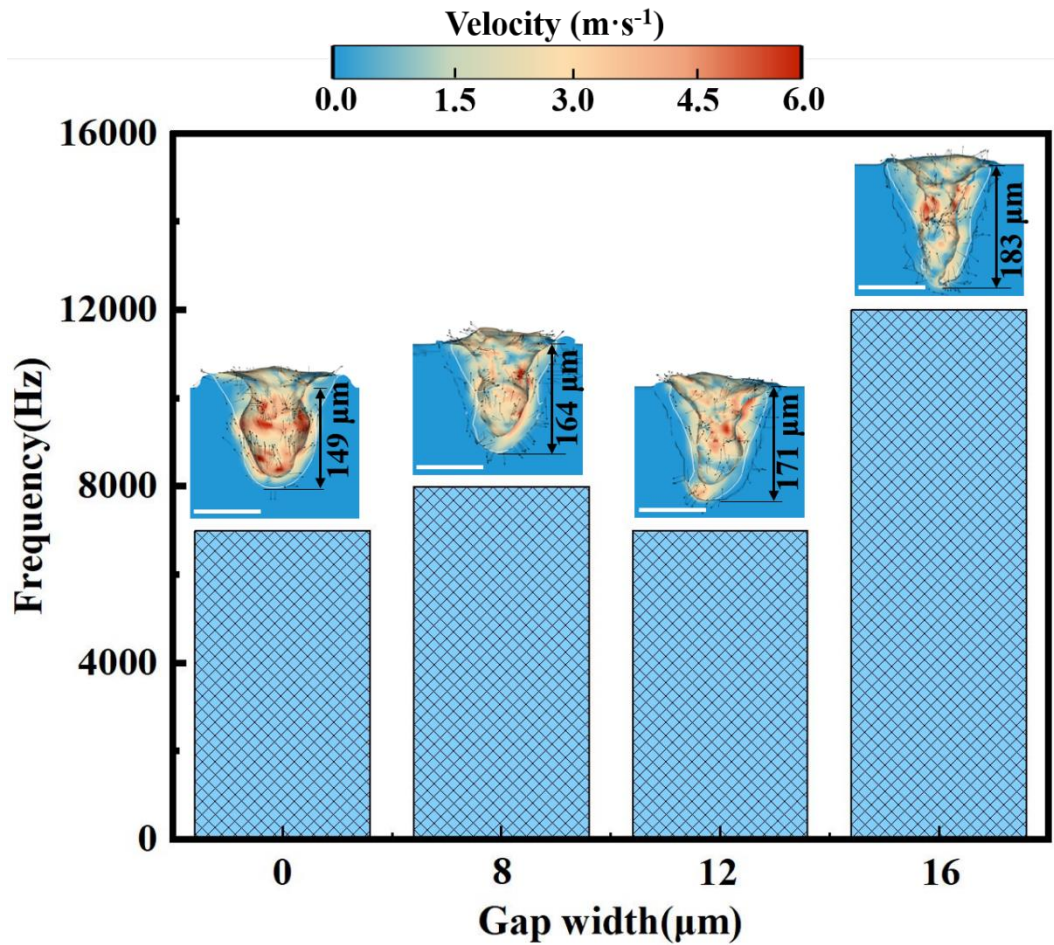
366

367 **Fig. 13** (a) Depth of molten pool with different gap values (0-16 μm) and (b) the
 368 enlarged part in the dotted box. (c) The molten pool profiles in the points of A-F. A and
 369 B represent the fluctuation of melt pool depth caused by the large gap; C-F indicate the
 370 perturbation to the melt pool due to the keyhole instability in all cases, resulting in great
 371 change in depth. The white dotted arrows indicate the necking.

372 As the moving speed of the laser in this model is slow ($16.7 \text{ mm} \cdot \text{s}^{-1}$), the generated

373 pores were mostly captured. Note that the simulation for larger number of pores in this
374 welding model is limited by our current disk memory. Here, we can still determine the
375 effect of gap on pore formation by the definition of bubble generation frequency,
376 namely, the bubble formation counts within one second.

377 **Fig. 14** shows there is little difference in the bubble formation frequency in the
378 cases of 0 μm , 8 μm and 12 μm . When the gap increases to 16 μm , the frequency
379 increases substantially. It is because of the special phenomenon of melt dropping down
380 to fill the gap in laser butt welding. Therefore, the generation of bubble depends on two
381 aspects. One is the velocity of the fluid flow. The more vigorous the flow, the easier it
382 is to generate pores. The other is the depth of gap filling. The greater the downward
383 filling, the more unstable the molten pool, and the higher chance to form a bubble. As
384 shown in **Fig. 12**, when the gap value is greater than 20 μm , the fluid falls down and
385 cannot even form a molten pool. In the case of 0 μm , there is no gap filling effect, and
386 the fluid velocity at the molten pool bottom is large, which causes bubbles due to the
387 fluctuation of the keyhole. As for the case of 8 μm , it possesses the advantages of low
388 heat dissipation and gap filling. Compared to 0 μm , the velocity decreases while the
389 melt pool depth increases. Under the effect of keyhole fluctuation and gap disturbance,
390 the frequency increases somewhat. In the case of 12 μm , despite of the increased molten
391 pool depth, the bubble frequency decreases slightly, which may be related to the further
392 reduced velocity compared to 8 μm . When it comes to the case of 16 μm , the frequency
393 is still high under the condition of large heat loss, which can be attributed to the
394 disturbance caused by the gap. Moreover, the gap filling effect results in an elongated
395 tip, which is likely to cause insufficient feeding at the bottom of the keyhole to form
396 pores. All in all, gap will disturb the stability of molten pool and promote pore
397 generation despite the heat loss.



398

399 **Fig. 14** Frequency of bubble generation with different gap values. The inserts show the
 400 fluid flow strength and gap filling degree corresponding to the gap below. It indicates
 401 strong flow for 0 μm, strong flow and weak downward filling for 8 μm, weak flow and
 402 weak downward filling for 12 μm, weak flow and strong downward filling for 16 μm.
 403 The scale bar is 100 μm.

404 **4. Conclusion**

405 In this paper, we developed a thermal-mechanistic-fluid coupled model to
 406 investigate the gap filling mechanism in laser butt welding of aluminum and the effects
 407 of gap on the molten pool characteristic and bubble generation. Our simulation model
 408 provided in-depth understanding of the experimental phenomenon of gap filling and
 409 bubble evolution obtained by in-situ X-ray imaging. Besides, the strategy to reduce the
 410 bubble defect in laser butt welding is suggested. The following key conclusions can be
 411 drawn:

- 412 (1) The metal melts and fills the gap due to the gravity and recoil pressure. Gap
 413 increases the heat dissipation. The competition between the solidification and melting
 414 determines the filling process and the shape of the molten pool. The gap filling effect

415 causes the molten pool tip to be elongated.

416 (2) Four phenomena appeared in sequence in the initial stage of butt welding. I.
417 Gap filling. The melting velocity exceeds the solidification velocity, the fluid flows
418 downward to fill the gap. II. Frozen. The solidification velocity dominates and the
419 molten pool bottom solidifies. III. Remelt. Heat accumulation results in the melting
420 process prevailing and the fluid continuously flows downward. IV. Bubble formation.
421 Necking occurs and promotes the keyhole fluctuation. Coupled with the tip elongated
422 effect, a bubble generates at the bottom of the keyhole.

423 (3) In the initial stable growth stage of the molten pool, the larger the gap width,
424 the deeper the molten pool, all of which is caused by the downward flow that fills the
425 gap. The sharp change of keyhole depth is due to the formation of necking, while the
426 small fluctuation of keyhole depth with larger gap values results from the gap
427 disturbance. The larger the gap, the earlier the gap perturbation occurs.

428 (4) The bubble formation depends on two aspects in laser butt welding due to its
429 unique phenomenon of melt dropping down to fill the gap. One is the degree of the
430 fluid flow and the other is gap filling. There is no big difference in the bubble formation
431 frequency when the gap is no more than 12 μm . When it increases to 16 μm , the
432 frequency increases substantially despite of the great heat loss. As the gap width
433 exceeds 20 μm , a continuous melt pool cannot be formed due to the fluid dropping
434 down, which is detrimental to the welding quality.

435 (5) In summary, it is proposed to minimize the gap width, such as reducing the
436 surface roughness, increasing the clamping force, and so on, to improve the joint quality
437 in the actual laser butt welding process.

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